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A quantum-kinetic equation for the description of internal dynamics of multilevel atomic systems moving through a target matter

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Abstract. The quantum mechanical consideration of a passage of relativistic elementary atoms (EA) through a target matter is given. A quantum-kinetic equation for the density matrix describing their internal state evolution at EA rest frame is derived.

1 Introduction

For the interpretation of the data of DIRAC experiment [1, 2] which aims to measure the lifetime of hydrogenlike EA consisting of π^+ and π^- mesons ($A_{2\pi}$ atoms) one needs to have the accurate theory for the description of internal dynamics of the $A_{2\pi}$ atoms moving through a target matter.

During their passage through the target $A_{2\pi}$ (pionium atoms) interacts with target atoms that causes the excitation, deexcitation or ionization of the $A_{2\pi}$. To describe these variations of $A_{2\pi}$ internal states the authors of [3] proposed a set of kinetic equations for the probabilities to find the pionium atom in the definite quantum state at some distance from the point of $A_{2\pi}$ production.

It is clear that such "classical" description is approximate because does not take into account the possible interference (quantum) effects. These last can be included in consideration only in the framework of density matrix formalism.

2 Derivation of a density matrix kinetic equation

The derivation of a kinetic equation for the density matrix of fast atomic systems passing through a target matter can be given at target rest frame [4], but more simple these equation can be obtained at rest frame of the EA.

At this frame the target moves with the velocity $\vec{v}_0$ and the electromagnetic field produced by target atoms is described by 4-vector potential $A_\mu = (\Phi, \vec{A})$, $\vec{A} = (\vec{v}_0/c)\Phi$.

The scalar potential Φ interacts with the charges of mesons and the vector potential A_μ with their currents. Because the typical velocities of the particles forming EA are of order $\alpha c \ll c$ (α is the fine structure constant), we will neglect the term proportional to the current in the Hamiltonian (see [5]).

Then internal dynamics of relativistic EA (later, for definiteness, "of pionium atoms") is described by the Schrödinger equation

$$i\frac{\partial\psi(\vec{r},t)}{\partial t} = H\psi(\vec{r},t) \tag{1}$$

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with the Hamiltonian of the form

$$H = H_0 + V(\vec{r}, t), \quad H_0 = T + V_0(\vec{r}) \tag{2}$$

and

$$T = -\Delta/2\mu = -(d/d\vec{r})^2/2\mu\,. \tag{3}$$

Here, $V_0(\vec{r})$ are the potential energy of pion-pion interaction and $V(\vec{r}, t)$ is the potential energy of interaction between the pionium and the target atom.

We will suppose that the positions of atoms inside the target are not varied during the interaction of target with the pionium atom (the so-called "frozen" target approximation). Then

$$V(\vec{r}) = e\sum_i [\Phi\left(\vec{r}_i(t) - \vec{r}/2\right) - \Phi\left(\vec{r}_i(t) + \vec{r}/2\right)]\,, \tag{4}$$

$$\vec{r}_i(t) = \vec{r}_i(t_0) + \vec{v}_0(t - t_0)\,, \tag{5}$$

$$\Phi(\vec{R}) = \gamma\Phi_0\sqrt{\vec{R}^2 + \gamma^2(\vec{v}_0\vec{R})^2}\,, \tag{6}$$

$$\vec{R} = \vec{r}_i(t) \mp \vec{r}/2, \quad \gamma = 1/\sqrt{1 - v_0^2/c^2}\,. \tag{7}$$

Here, Φ_0 is the potential of the target atom at it's rest frame, and we have put the origin of the coordinate system to the center-of-mass of pionium.

Thus, the solution of the Schrödinger equation (1) depends on "frozen" positions $\vec{r}_i(t_0)$ of the target atoms

$$\psi(\vec{r}, t) = \psi\Big(\vec{r}, t; \{\vec{r}_i(t_0)\}\Big)\,.$$

The density matrix of pionium is defined as follows:

$$\rho(\vec{r}, \vec{r}'; t) \;\; = \;\; \Big\langle \psi\Big(\vec{r}, t; \{\vec{r}_i(t_0)\}\Big) \cdot \psi(\vec{r}', t; \{\vec{r}_i(t_0)\}) \Big\rangle_{\{\vec{r}_i(t_0)\}}\,, \tag{8}$$

where $\langle\rangle_{\{\vec{r}_i(t_0)\}}$ means averaging over all possible positions of target atoms.

Let t_0 be the point of time when moving target meet the pionium atom and $\psi(\vec{r}, t_0)$ is the value of pionium wave function at this time. Then at $t > t_0$

$$\psi\Big(\vec{r}, t; \{\vec{r}_i(t_0)\}\Big) = \int G\Big(\vec{r}, \vec{r}_0; t, t_0; \{\vec{r}_i(t_0)\}\Big)\psi_i(\vec{r}_0, t_0)d\vec{r}_0\,, \tag{9}$$

where G is the Green function of Eq. (1).

According to [6], it can be expressed in terms of the path integral

$$G(\vec{r}, \vec{r}_0; t, t_0; \{\vec{r}_i(t_0)\}) = \int D\vec{r}(t)\exp(iS)\,, \tag{10}$$

with

$$S = S_0 + S_1\,, \tag{11}$$

$$S_0 = \int\limits_{t_0}^{t} dt' L_0(\vec{v}(t'), \vec{r}(t'))\,, \quad S_1 = -\int\limits_{t_0}^{t} dt' V(\vec{r}(t'), t')\,, \tag{12}$$

$$L_0(\vec{v}(t'), \vec{r}(t')) \;=\; \mu\vec{v}^{\,2}(t')/2 - V_0(\vec{r}(t'))\,, \tag{13}$$

$$\vec{v}(t') = d\vec{r}(t')/dt'\,.$$

It can be shown (see [9]) that

$$S_1 \;=\; -\sum_i \left\{\chi\Big(\vec{b}_i + \vec{s}(t_i)/2\Big) - \chi\Big(\vec{b}_i - \vec{s}(t_i)/2\Big)\right\}\vartheta(t - t_i)\,, \tag{14}$$

where

$$\chi(\vec{b}_\pm) = \frac{e}{v_0}\int\limits_{-\infty}^{\infty} \Phi\left(\sqrt{\vec{b}_\pm^{\,2} + z^2}\right) dz\,, \tag{15}$$

$$\vec{b}_\pm = \vec{b}_i \pm \frac{\vec{s}(t_i)}{2}, \quad t_i = t_0 + \frac{\vec{v}_0 \cdot \vec{r}_i(t_0)}{v_0^2}\,, \tag{16}$$

$$\vec{b}_i \;=\; \vec{r}_i(t_0)_\perp = \vec{r}_i(t_0) - \frac{\vec{v}_0 \cdot \vec{r}_i(t_0)}{v_0^2} \cdot \vec{v}_0\,, \tag{17}$$

$$\vec{s}(t_i) \;=\; \vec{r}(t_i)_\perp = \vec{r}(t_i) - \frac{\vec{v}_0 \cdot \vec{r}_i(t_0)}{v_0^2} \cdot \vec{v}_0\,, \tag{18}$$

the Heavyside step function $\vartheta(t)$ is 0 for $t < 0$ and 1 for $t > 0$.

Substituting (10)-(18) into (8) and performing the averaging over the "frozen" positions of target atoms with the help of the prescription of [7, 8], one can get the following representation for the density matrix:

$$\rho(\vec{r}, \vec{r}'; t) = \int \widetilde{G}(\vec{r}, \vec{r}'; \vec{r}_0, \vec{r}_0'; t, t_0)\psi_i(\vec{r}_0, t_0)\psi_i^*(\vec{r}_0', t_0) d\vec{r}_0 d\vec{r}_0'\,, \tag{19}$$

with

$$\widetilde{G}(\vec{r}, \vec{r}'; \vec{r}_0, \vec{r}_0'; t, t_0) = \int D\vec{r}(t) D\vec{r}'(t) \exp(i\widetilde{S}_0 - W)\,, \tag{20}$$

$$\widetilde{S}_0 \;=\; \int\limits_{t_0}^{t} dt' \left\{L_0(\vec{v}(t'), \vec{r}(t')) - L_0(\vec{v}'(t'), \vec{r}'(t'))\right\}\,, \tag{21}$$

$$W \;=\; v_0\gamma n_0 \int\limits_{t_0}^{t} dt' \Omega(\vec{s}(t'), \vec{s}'(t'))\,, \tag{22}$$

$$\Omega(\vec{s}(t'), \vec{s}'(t')) \;=\; \int d^2b \left\{1 - \exp\Big(i\Phi(\vec{b}, \vec{s}(t'), \vec{s}'(t'))\Big)\right\}\,, \tag{23}$$

$$\Phi(\vec{b},\vec{s}(t'),\vec{s}'(t')) = \chi(\vec{b}+\vec{s}(t')/2)-\chi(\vec{b}-\vec{s}(t')/2) - \chi(\vec{b}+\vec{s}'(t')/2)+(\vec{b}-\vec{s}'(t')/2)\,. \quad (24)$$

Here, n_0 is the number of atoms in the unite volume of target at it's rest frame, $\vec{s}$ and $\vec{s}'$ are the transverse parts of the vectors $\vec{r}$ and $\vec{r}'$.

From Eqs. (19)-(22) it easily derive (see [6]) the following equation for the density matrix:

$$i\frac{\partial\rho(\vec{r},\vec{r}';t)}{\partial t} = H_0(\vec{r})\rho(\vec{r},\vec{r}';t) - H_0(\vec{r}')\rho(\vec{r},\vec{r}';t) -iv_0\gamma n_0\Omega(\vec{s},\vec{s}')\rho(\vec{r},\vec{r}';t)\,, \quad (25)$$

where the last operator term describes the Coulomb interaction between EA and the target atoms with account of all multiphoton exchanges. Using a generalized optical potential of the form $V_{opt}(\vec{s},\vec{s}') = k\Omega(\vec{s},\vec{s}')$, where $k = -iv_0\gamma n_0$, we can represent this term as $V_{opt}\rho(t)$.

The form of Eq. (25) is similar to the form of Eq. (116) in Ref. [10] describing the internal dynamics of multilevel atoms in laser fields, where the last term $\Gamma\rho$ describes the contribution of the spontaneous relaxation.

The equations of motion for the density matrix elements

$$\rho_{ik} = \int \psi_i^*(\vec{r})\psi_k(\vec{r}')\rho(\vec{r},\vec{r}')d\vec{r}d\vec{r}' \quad (26)$$

looks like as follows:

$$\frac{\partial\rho_{ik}(t)}{\partial t} = i\Delta_{ik}\rho_{ik}(t) - v_0\gamma n_0\sum_{l,m}\Omega_{ik,lm}\rho_{lm}(t)\,, \quad (27)$$

where

$$\Delta_{ik} = \varepsilon_k - \varepsilon_i\,,$$
$$\Omega_{ik,lm} = \int \psi_i^*(\vec{r})\psi_l(\vec{r})\psi_k(\vec{r}')\psi_m^*(\vec{r}')\Omega(\vec{s},\vec{s}')d\vec{r}d\vec{r}'\,, \quad (28)$$

the EA wave functions $\psi_{i(k)}$ and binding energies $\varepsilon_{i(k)}$ obey the Schrödinger equation

$$H_0\psi_{i(k)} = \varepsilon_{i(k)}\psi_{i(k)}\,. \quad (29)$$

Taking into account the lifetime τ_i of the EA, we can obtain

$$\frac{\partial\rho_{ik}(t)}{\partial t} = \left[i(\varepsilon_k-\varepsilon_i) - \frac{1}{2}(\Gamma_i+\Gamma_k)\right]\rho_{ik}(t) - v_0\gamma n_0\sum_{l,m}\Omega_{ik,lm}\rho_{lm}(t)\,, \quad (30)$$

where $\Gamma_{i(k)} = 1/\tau_{i(k)}$ is the EA levels width (for details see [4]).

Properties of the solution of (25) will be discussed in the following paper.

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